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14. ABSTRACT
We study optical lattice systems, in which rapid experimental progress and tremendous potential for quantum emulations provide many opportunities for investigating open questions in condensed matter physics, and possibly quantum computing. We study the many-body effects in two- and three-dimensional Hubbard-like models, focusing on long-wavelength collective modes, such as spin-density waves, and

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Report Title

Final Report: Fermionic Optical Lattices: A Computational Study

ABSTRACT

We study optical lattice systems, in which rapid experimental progress and tremendous potential for quantum emulations provide many opportunities for investigating open questions in condensed matter physics, and possibly quantum computing. We study the many-body effects in two- and three-dimensional Hubbard-like models, focusing on long-wavelength collective modes, such as spin-density waves, and other matter-wave properties resulting from particle interaction and quantum coherence. The second focus is on molecular physics, where we aim to achieve an accurate, robust many-body paradigm for predicting properties and mechanisms of small molecules. Success of the research can contribute a powerful and yet heretofore largely missing third (computational) component for these areas, and help accelerate the realization of novel applications and new technological capabilities of interest to the Army and beyond.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
08/23/2012	1.00	J. Carlson, Stefano Gandolfi, Kevin Schmidt, Shiwei Zhang. Auxiliary-field quantum Monte Carlo method for strongly paired fermions, Physical Review A, (12 2011): 0. doi: 10.1103/PhysRevA.84.061602
08/23/2012	5.00	A. Euverte, F. Hébert, S. Chiesa, R. Scalettar, G. Batrouni. Kondo Screening and Magnetism at Interfaces, Physical Review Letters, (06 2012): 0. doi: 10.1103/PhysRevLett.108.246401
08/23/2012	4.00	Chia-Chen Chang, Shiwei Zhang, David Ceperley. Itinerant ferromagnetism in a Fermi gas with contact interaction: Magnetic properties in a dilute Hubbard model, Physical Review A, (12 2010): 0. doi: 10.1103/PhysRevA.82.061603
08/23/2012	3.00	S. Zhou, D. Ceperley, Shiwei Zhang. Validity of the scattering-length approximation in strongly interacting Fermi systems, Physical Review A, (07 2011): 0. doi: 10.1103/PhysRevA.84.013625
08/23/2012	2.00	Jie Xu, Chia-Chen Chang, Eric J Walter, Shiwei Zhang. Spin- and charge-density waves in the Hartree–Fock ground state of the two-dimensional Hubbard model, Journal of Physics: Condensed Matter, (12 2011): 0. doi: 10.1088/0953-8984/23/50/505601
09/12/2013	6.00	Brenda M. Rubenstein, Shiwei Zhang, David R. Reichman. Finite-temperature auxiliary-field quantum Monte Carlo technique for Bose-Fermi mixtures, Physical Review A, (11 2012): 0. doi: 10.1103/PhysRevA.86.053606
10/22/2014	8.00	Jie Xu, Simone Chiesa, Eric J Walter, Shiwei Zhang. Magnetic order in the Hubbard model in three dimensions and the crossover to two dimensions, Journal of Physics: Condensed Matter, (10 2013): 0. doi: 10.1088/0953-8984/25/41/415602
10/22/2014	9.00	Simone Chiesa, Shiwei Zhang. Phases of attractive spin-imbalanced fermions in square lattices, Physical Review A, (10 2013): 0. doi: 10.1103/PhysRevA.88.043624

TOTAL: **8**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received	Paper

TOTAL:

Number of Manuscripts:

Books

Received	Book

TOTAL:

Received		Book Chapter
09/12/2013	7.00	Shiwei Zhang. Auxiliary-Field Quantum Monte Carlofor Correlated Electron Systems, Forschungszentrum Julich: E. Pavarini, E. Koch, and U. Schollwock, (09 2013)

TOTAL: **1**

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Simone Chiesa	0.35
FTE Equivalent:	**0.35**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

All previous activities and accomplishments have been reported in the interim reports. This grant was on a small modification last year to help support a postdoctoral scientist to finish two projects already underway. The projects have been reported last year. We summarize these below.

Magnetic order in the repulsive Fermi-Hubbard model in three-dimensions and the crossover to two-dimensions. Systems of fermions described by the three-dimensional (3D) repulsive Hubbard model on a cubic lattice have recently attracted considerable attention due to their possible experimental realization via cold atoms in an optical lattice. Because analytical and numerical results are limited away from half-filling, we study the ground state of the doped system from weak to intermediate interaction strengths within the generalized Hartree-Fock approximation. The exact solution to the self-consistent-field equations in the thermodynamic limit is obtained and the ground state is shown to exhibit antiferromagnetic order and incommensurate spin-density waves (SDW). At low interaction strengths, the SDW has unidirectional character with a leading wave-vector along the $<100>$-direction, and the system is metallic. As the interaction increases, the system undergoes a simultaneous structural and metal-to-insulator transition to a unidirectional SDW state along the $<111>$-direction, with a different wavelength. We systematically determine the real- and momentum-space properties of these states. The crossover from 3D to two-dimensions (2D) is then studied by varying the inter-plane hopping amplitude, which can be experimentally realized by tuning the distance between a stack of square-lattice layers. Detailed comparisons are made between the exact numerical results and predictions from the pairing model, a variational {\em ansatz} based on the pairing of spins in the vicinity of the Fermi surface. Most of the numerical results can be understood quantitatively from the ansatz, which provides a simple picture for the nature of the SDW states.

Phases of attractive spin-imbalanced fermions in square optical lattices. We determine the relative stability of different ground-state phases of spin-imbalanced popula- tions of attractive fermions in square lattices. The phases are systematically characterized by the symmetry of the order parameter and the real- and momentum-space structures using Hartree- Fock-Bogoliubov theory. We find several type of unidirectional Larkin-Ovchinikov-type phases. We discuss the effect of commensuration between the ordering wave vector and the density imbalance, and describe the mechanism of Fermi surface reconstruction and pairing for various orders. A robust supersolid phase is shown to exist when the ordering wave vector is diagonally directed.

Technology Transfer